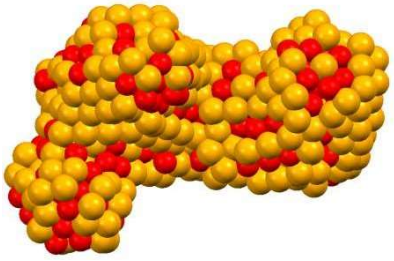
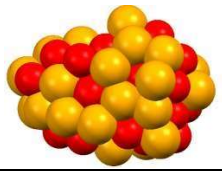
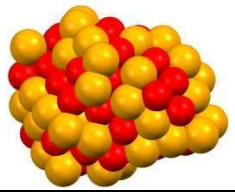
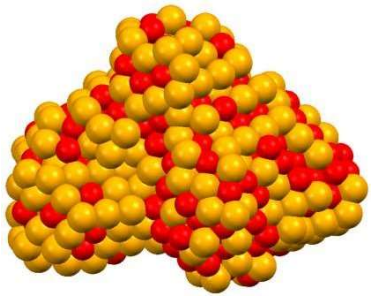
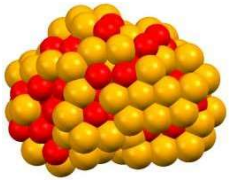
Supporting Information:

Table S1. The no. of different atoms, mole fractions, and percent of the surface atoms for the clusters formed at x_{Au}= 0.5 and 300 K and 1 bar (Au is in yellow, Ir is in red).

Time (ns)	$Au_{0.5}Ir_{0.5}$ Nanoalloy	N_{tot}	N_{Au}	N_{Ir}	X_{Au}	X_{Ir}	N_{Surf} Au	N_{Surf} Ir	$\%N_{Surf}$ Au	$\%N_{surf}$ Ir
3		710	364	346	0.51	0.49	273	134	67.0762	32.923
3		61	33	28	0.54	0.46	31	18	63.2653	36.734
3		110	56	54	0.51	0.49	45	35	56.25	43.75
3		572	272	300	0.48	0.52	193	118	62.0579	37.942
3		182	93	89	0.51	0.49	78	42	65	35

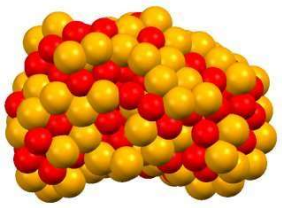
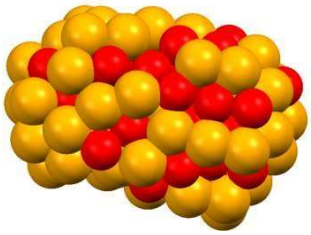
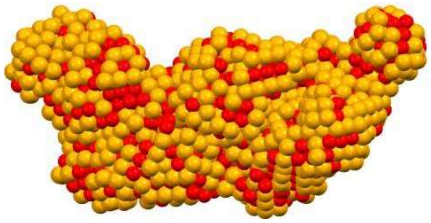
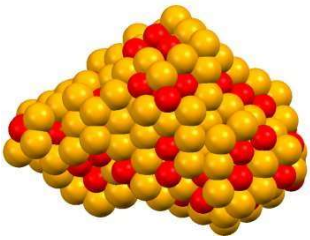
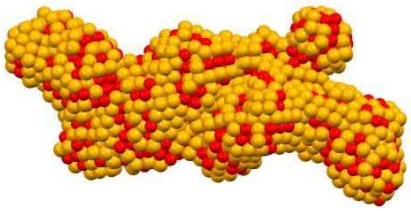
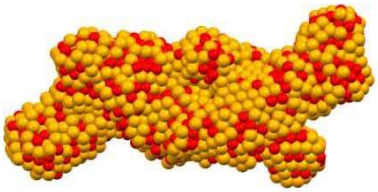
3		242	118	124	0.49	0.51	94	60	61.0389	38.9611
3		123	64	59	0.52	0.48	57	29	66.2791	33.7209
4		1648	826	822	0.50	0.50	581	307	65.4279	34.5721
4		352	174	178	0.49	0.51	126	83	60.2871	39.7129
6		2000	1000	1000	0.50	0.50	670	336	66.6	33.4
20		2000	1000	1000	0.50	0.50	674	331	67.0647	32.9353

Table S2. Same as Table 1 but at 100 bar.

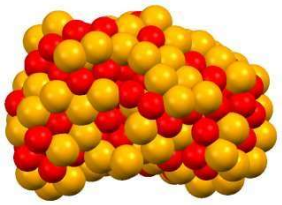
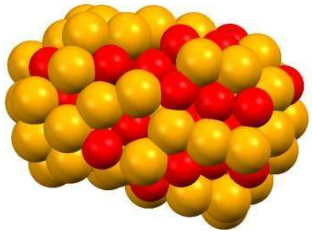
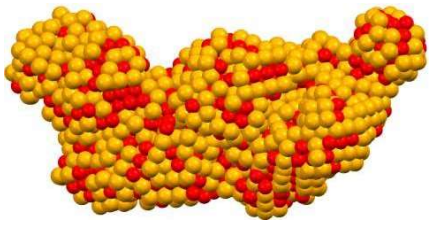
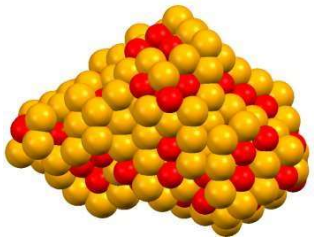
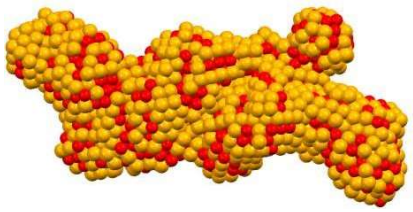
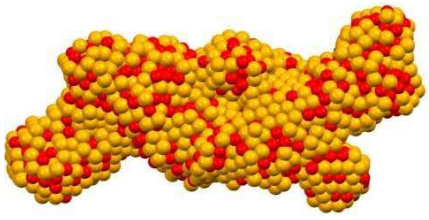
3		242	118	124	0.49	0.51	94	60	61.0389	38.9611
3		123	64	59	0.52	0.48	57	29	66.2791	33.7209
4		1648	826	822	0.50	0.50	581	307	65.4279	34.5721
4		352	174	178	0.49	0.51	126	83	60.2871	39.7129
6		2000	1000	1000	0.50	0.50	670	336	66.6	33.4
20		2000	1000	1000	0.50	0.50	674	331	67.0647	32.9353

Table S3. Same as Table 1, but at x_{Au}=0.25.

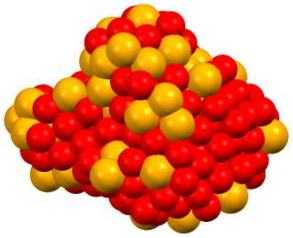
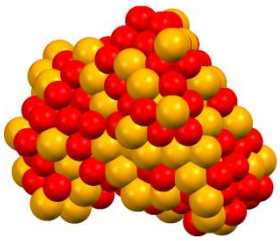
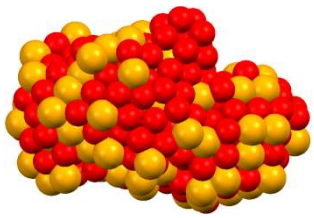
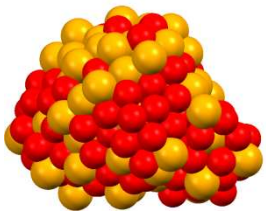
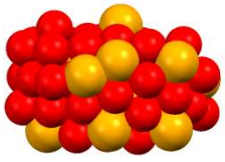
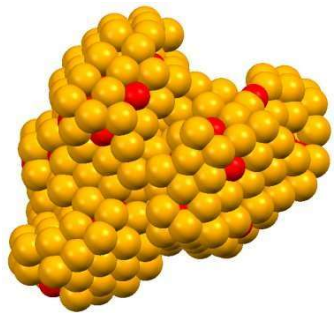
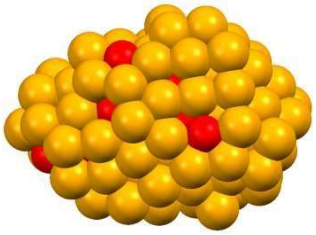
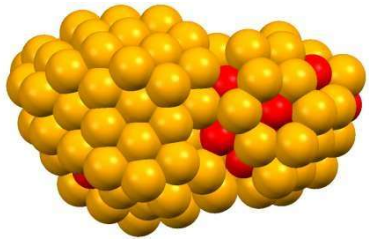
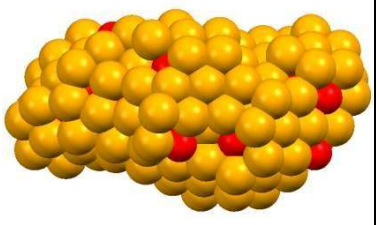
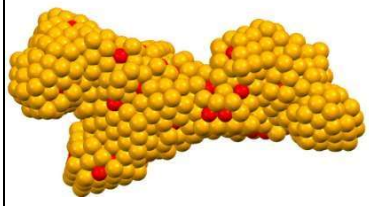
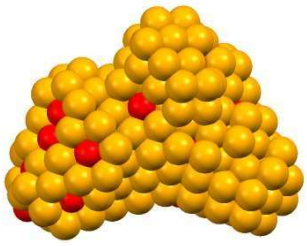
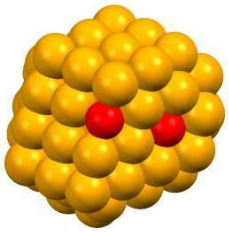
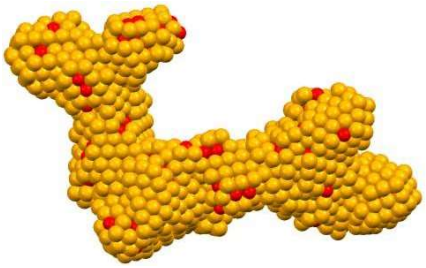
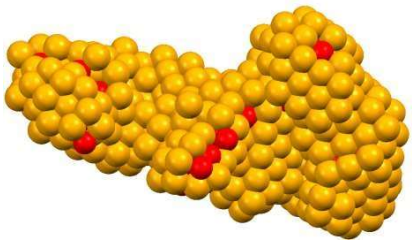
Time (ns)	$Au_{0.25}$ $Ir_{0.75}$ Nanoalloy	N_{tot}	N_{Au}	N_{Ir}	X_{Au}	X_{Ir}	N_{Surf} Au	N_{Surf} Ir	$\%N_{surf}$ Ir	$\%N_{Surf}$ Au
3		238	56	182	0.24	0.76	43	109	71.7105	28.2895
3		278	77	201	0.28	0.72	60	117	66.1017	33.8983
3		300	86	214	0.29	0.71	70	124	63.9175	36.0825
3		208	58	150	0.28	0.72	52	85	62.0438	37.9562
3		64	16	48	0.25	0.75	12	39	76.4706	23.5294

Table S4. Same as Table 1, but at x_{Au}=0.75.

Time (ns)	$Au_{0.75}Ir_{0.25}$ Nanoalloy	N_{tot}	N_{Au}	N_{Ir}	x_{Au}	x_{Ir}	N_{Surf} Au	N_{Surf} Ir	$\%N_{Surf}$ Au	$\%N_{surf}$ Ir
3		361	270	91	0.75	0.25	218	21	91.213	8.786
3		139	107	32	0.77	0.33	88	8	91.666	8.333
3		155	106	49	0.68	0.32	94	15	86.238	13.761
3		174	135	39	0.78	0.22	119	9	92.968	7.031

3		821	617	204	0.75	0.25	450	31	93.555	6.445

3		257	195	62	0.76	0.24	155	18	89.595	10.4046
3		93	70	23	0.75	0.25	61	6	91.0448	8.9552
4		1465	1095	370	0.75	0.25	761	70	91.5764	8.4236
4		535	405	130	0.75	0.25	335	28	92.2865	7.7135

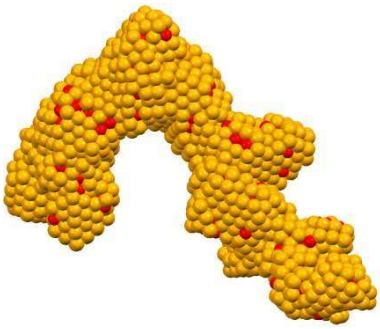
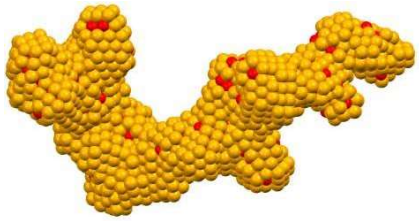
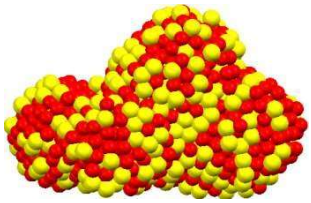
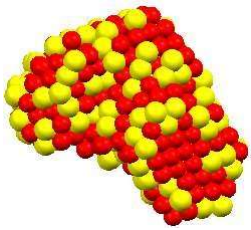
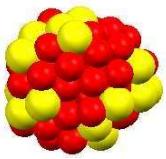
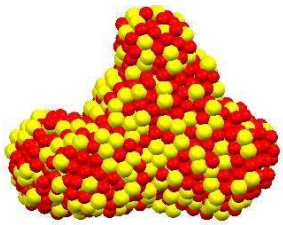
6		2000	1500	500	0.75	0.25	1051	90	92.1122	7.8878
20		2000	1500	500	0.75	0.25	1026	83	92.5158	7.4842

Table S5. Same as Table 1, but at x_{Au}= 0.25 and 1000 K.

Time (ns)	$Au_{0.25}Ir_{0.75}$ Nanoalloy	N_{tot}	N_{Au}	N_{Ir}	X_{Au}	X_{Ir}	N_{Surf} Au	N_{Surf} Ir	$\%N_{Surf}$ Au	$\%N_{surf}$ Ir
3		1370	336	1034	0.25	0.75	230	412	35.8255	64.1745
3		555	143	412	0.26	0.74	110	203	35.1438	64.8562
3		75	21	54	0.28	0.72	20	37	35.0877	64.9123
4		1445	357	1088	0.25	0.75	242	425	36.2819	63.7181
4		555	143	412	0.26	0.74	111	204	35.2381	64.7619

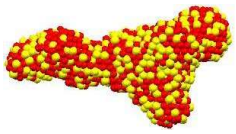
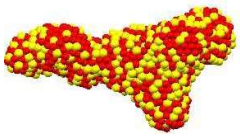
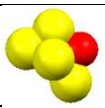
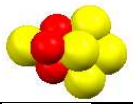
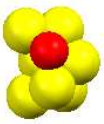
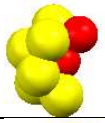
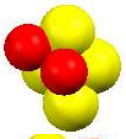
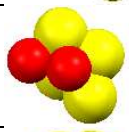
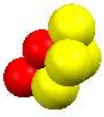
6		2000	500	1500	0.25	0.75	350	605	36.6492	63.3508
20		2000	500	1500	0.25	0.75	340	595	36.3636	63.6364

Table S6. The no. of different atoms and mole fractions formed at x_{Au}=0.75 and T= 300 K and P=1 in early stages of the condensation process (Au is in yellow, Ir is in red).

t (ns)	$Au_{0.75}Ir_{0.25}$ **Nanoalloy**	N_{tot}	N_{Au}	N_{Ir}	X_{Au}	X_{Ir}
2		6	4	2	0.67	0.33
		16	8	8	0.50	0.50
		7	2	5	0.29	0.71
		10	6	4	0.60	0.40
		6	3	3	0.50	0.50
		7	1	6	0.14	0.86
		8	7	1	0.87	0.13
		8	6	2	0.75	0.25
		6	4	2	0.67	0.33
		6	5	1	0.83	0.17
		6	4	2	0.67	0.33
		10	7	3	0.70	0.30
		6	4	2	0.67	0.33
		6	4	2	0.67	0.33
		5	4	1	0.8	0.2

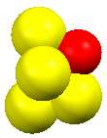
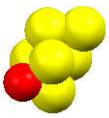
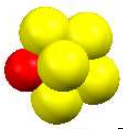
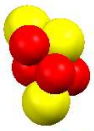
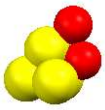
		7	4	3	0.57	0.43
		6	5	1	0.83	0.17
		6	1	5	0.17	0.83
		8	6	2	0.75	0.25
		7	6	1	0.86	0.14
		7	5	2	0.71	0.29
		7	5	2	0.71	0.29
		7	3	4	0.43	0.57
		6	4	2	0.67	0.33
		8	8	0	0.100	0
		8	3	5	0.38	0.62
		6	6	0	0.100	0
		12	9	3	0.75	0.25
		6	5	1	0.83	0.17

Table S7. The formed core-shell structures during the smaller simulation times (before the coalescence)

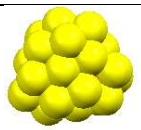
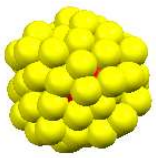
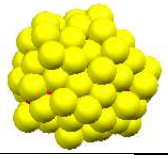
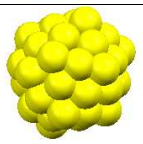
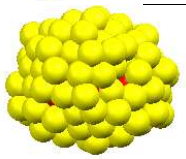
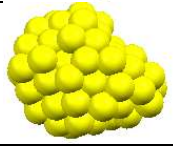
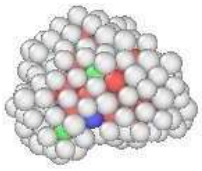
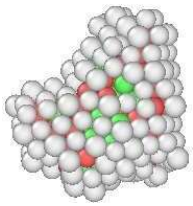
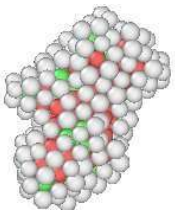
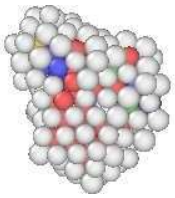
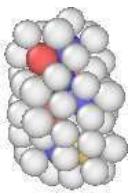
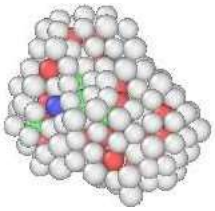
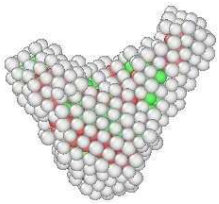
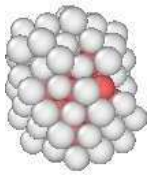
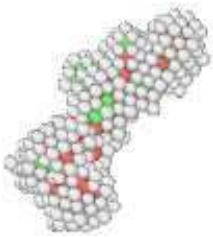
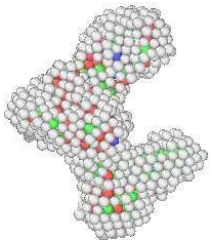
T (K)	P (bar)		N_{tot}	N_{Au}	N_{Ir}	$N_{Surf\ Au}$	$N_{Surf\ Ir}$
300	10		27	24	3	24	0
300	10		13	12	1	12	0
300	50		80	68	12	59	0
300	50		19	17	2	17	0
300	50		16	15	1	15	0
500	1		92	76	16	64	0
500	1		41	35	6	34	0
500	1		17	16	1	16	0
500	1		14	13	1	13	0
500	50		47	40	7	38	0
500	100		156	122	34	98	0
500	100		83	71	12	61	0

Table S8. The percentage of fcc hcp, bcc, and ico atoms (ordered atoms) and other atoms (disordered atoms) in the different nanoclusters at x_{Au}=0.25 and 300 K and 1 bar.

Time (ns)	$Au_{0.25}Ir_{0.75}$ Nanoalloy	N_{tot}	% fcc	% hcp	% bcc	% ico	% other
3		238	2.5	32.4	3.4	1.7	60.1
3		278	12.6	30.6	0.0	0.0	56.8
3		300	11.3	29.0	0.0	0.3	59.3
3		208	2.4	21.2	9.6	2.4	64.4
3		64	0.0	7.8	7.8	3.1	81.3

3		237	3.4	27.4	1.7	0.0	67.5
3		571	17.9	24.5	0.0	0.2	57.4
3		104	2.9	23.1	1.9	0.0	72.1
4		578	12.8	31.3	0.3	0.2	55.4
4		1422	14.5	34.2	1.7	0.3	49.3

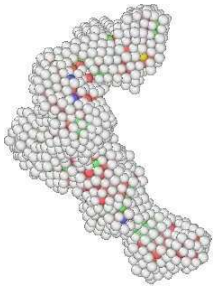
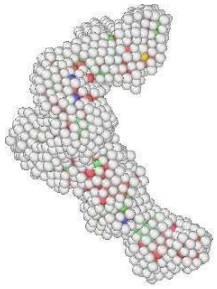
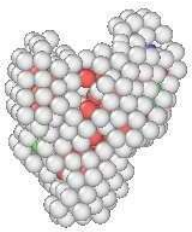
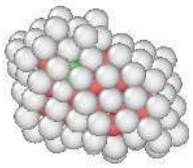
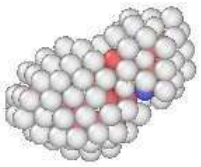
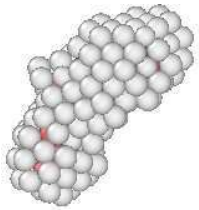
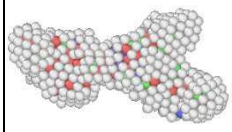
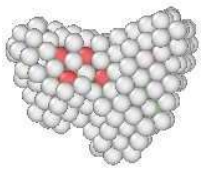
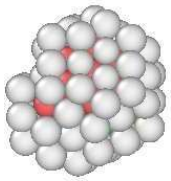
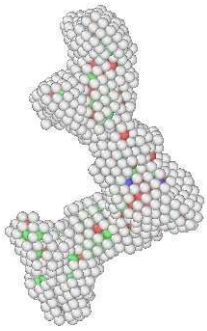
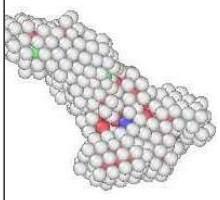
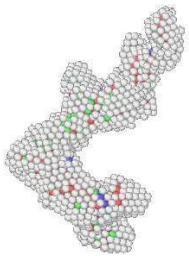
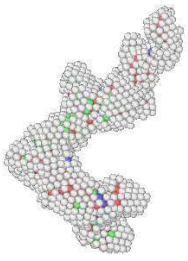
6		2000	15.2	33.3	2.1	0.3	49.1
20		2000	16.4	24.6	1.1	0.1	57.8

Table S9. The percentage of fcc hcp, bcc, and ico atoms (ordered atoms) and other atoms (disordered atoms) in the different nanoclusters at x_{Au}=0.75 and 300 K and 1 bar.

Time (ns)	$Au_{0.75}Ir_{0.25}$ Nanoalloy	N_{tot}	% fcc	% hcp	% bcc	% ico	% other
3		361	12.2	24.7	1.1	0.0	60.2
3		139	2.2	32.4	0.0	0.7	64.7
3		155	0.0	28.4	2.6	0.6	68.4
3		174	10.3	18.4	0.6	0.0	70.7
3		821	10.6	28.3	3.3	0.1	57.7

3		257	14.8	21.0	0.0	0.4	63.8
3		93	7.5	21.5	0.0	0.0	71.0
4		1465	12.7	23.1	2.1	0.1	61.9
4		535	12.0	23.9	0.7	0.0	63.4
6		2000	17.1	27.1	1.6	0.1	54.0
20		2000	16.8	27.3	0.8	0.1	55.0

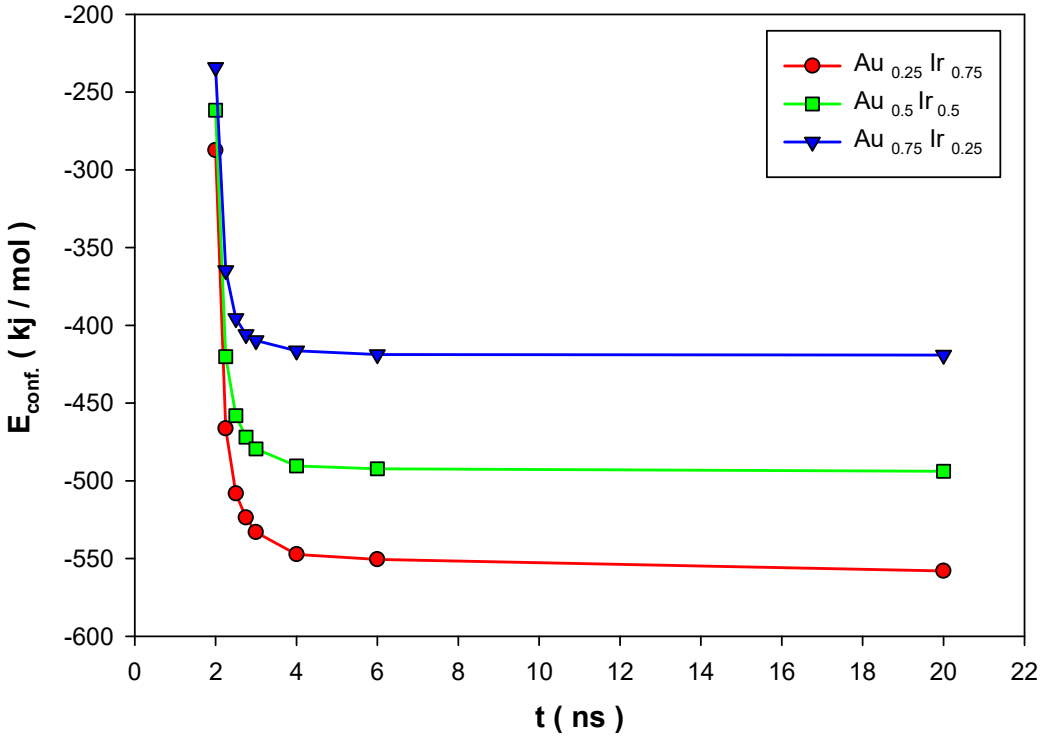


Fig S1. The configurational energy of the systems at 300 K and 1 bar and the different simulation times.

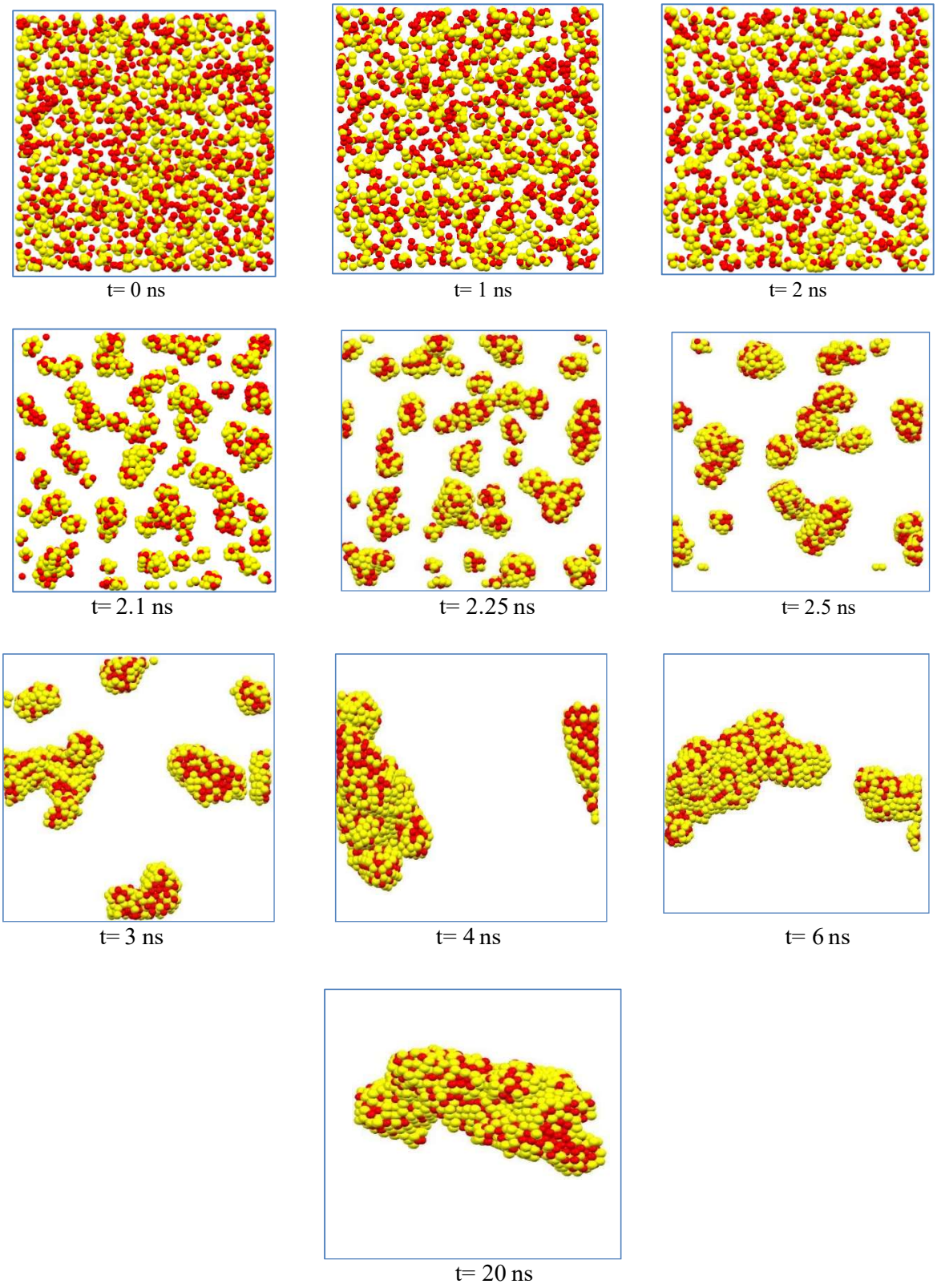


Fig S2. The snapshots of the formed clusters at x_{Au}= 0.5 at 300 K and 1 bar the different simulation times (Au is in yellow and Ir is in red). The Ar atoms have been deleted for clarity.

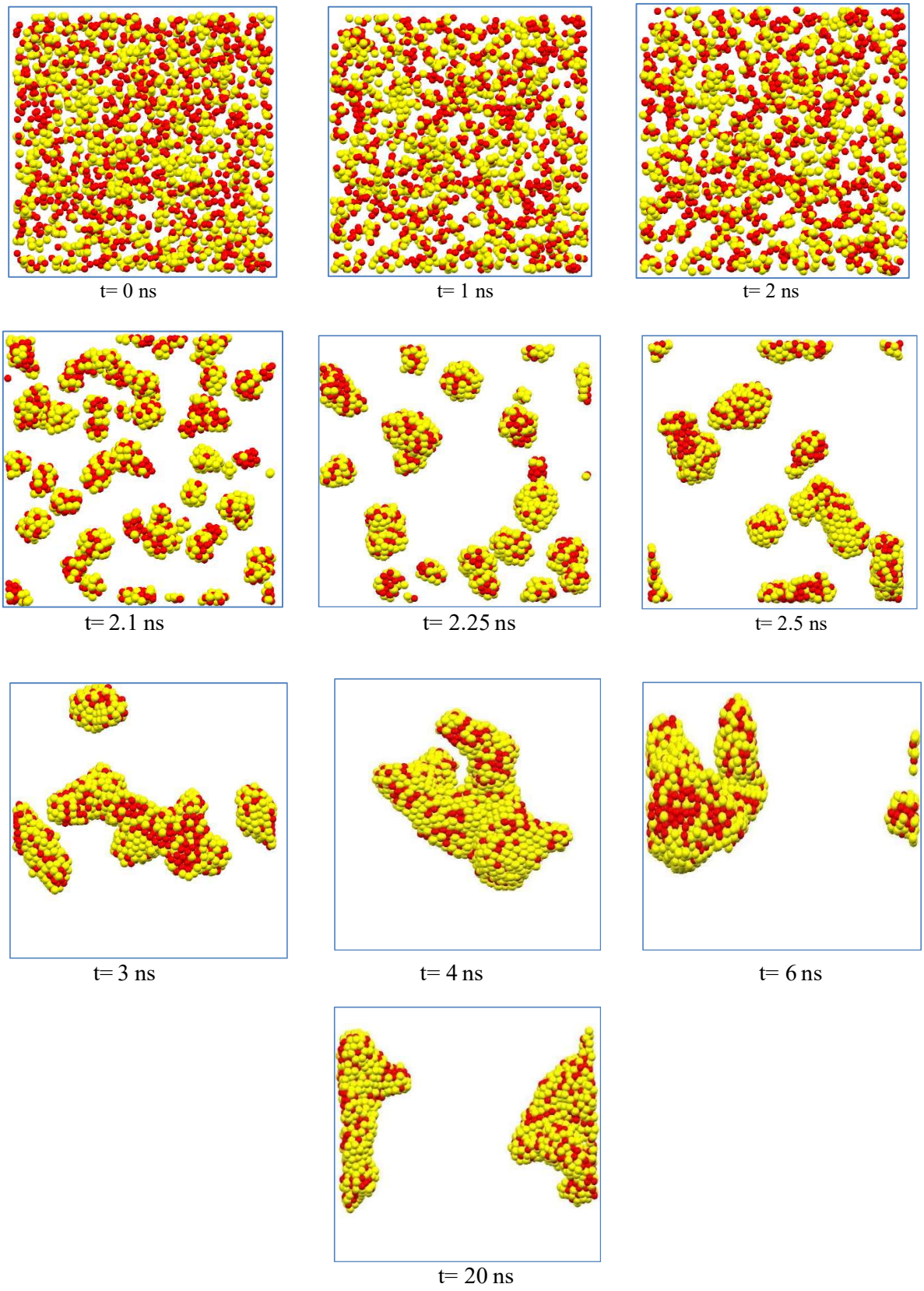
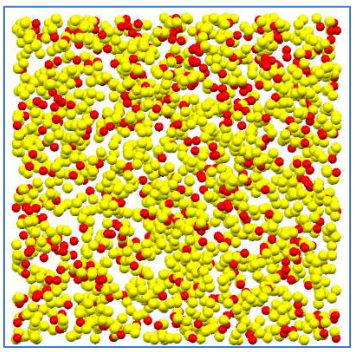
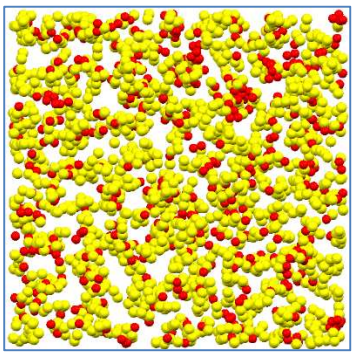


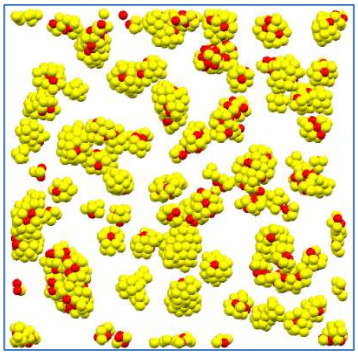
Fig. S3. The same as Fig. S1, but at 100 bar



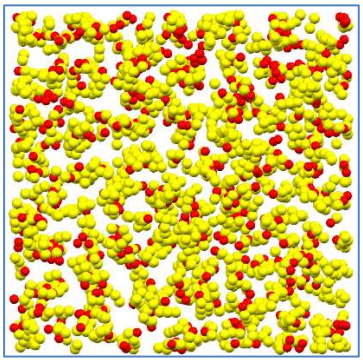
t= 0 ns



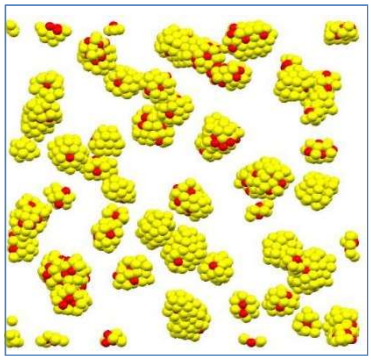
t= 1 ns



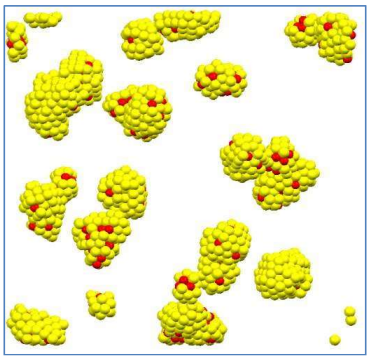
t= 2 ns



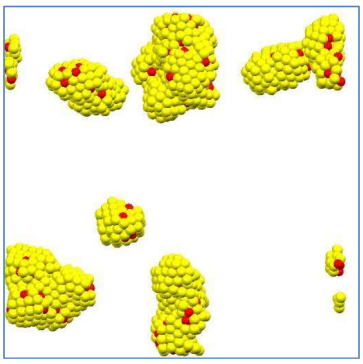
t= 2.1 ns



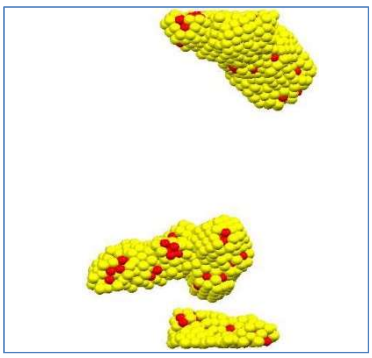
t= 2.25 ns



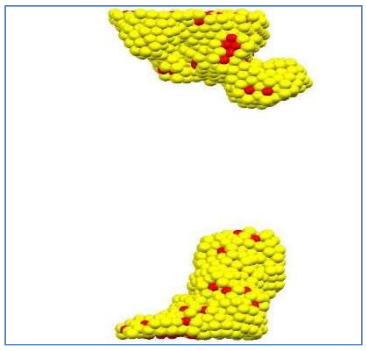
t= 2.5 ns



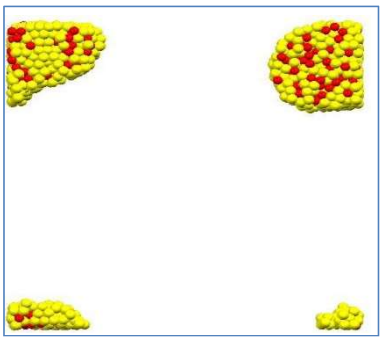
t= 3 ns



t= 4 ns

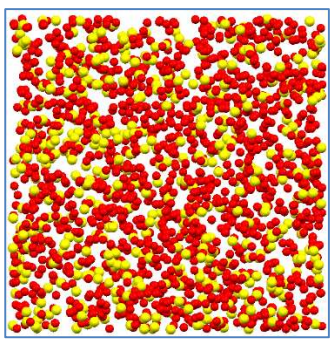


t= 6 ns

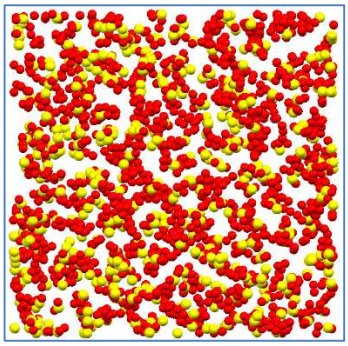


t= 20 ns

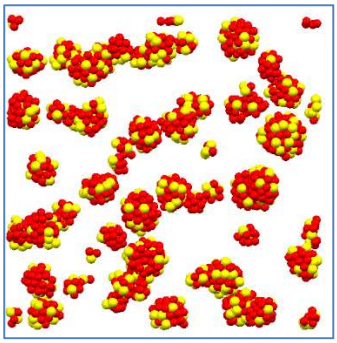
Fig. S4. The same as Fig. S1, but at x_{Au}=0.75.



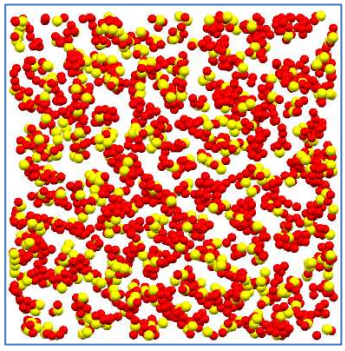
t= 0 ns



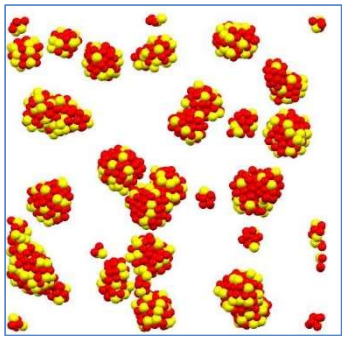
t= 1 ns



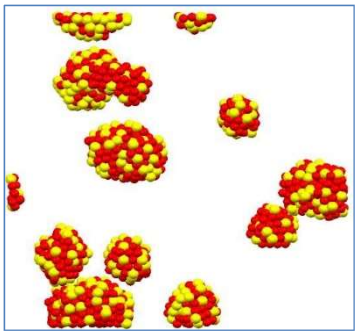
t= 2 ns



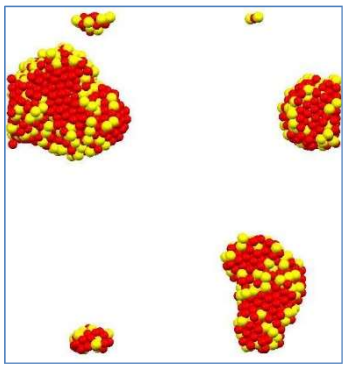
t= 2.1 ns



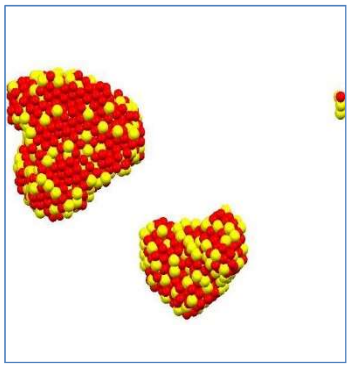
t= 2.25 ns



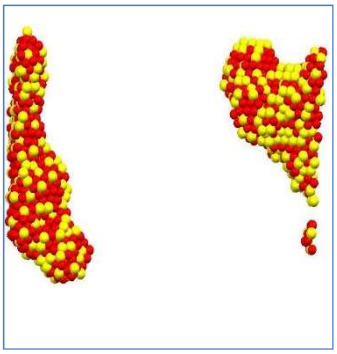
t= 2.5 ns



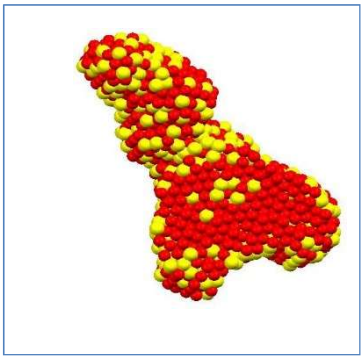
t= 3 ns



t= 4 ns

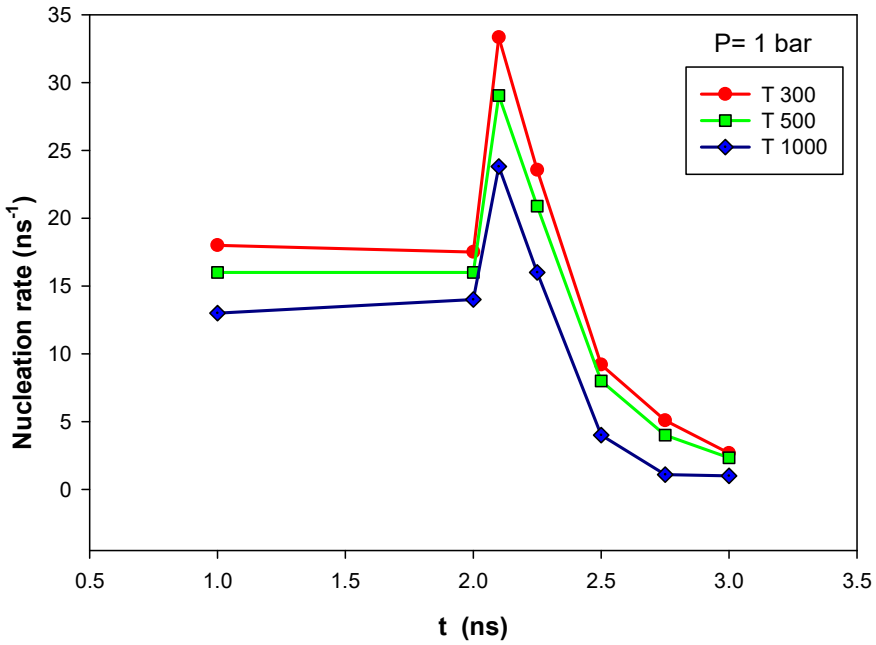


t= 6 ns



t= 20 ns

Fig S5. The same as Fig. S1, but at x_{Au}=0.25 and T= 1000 K.



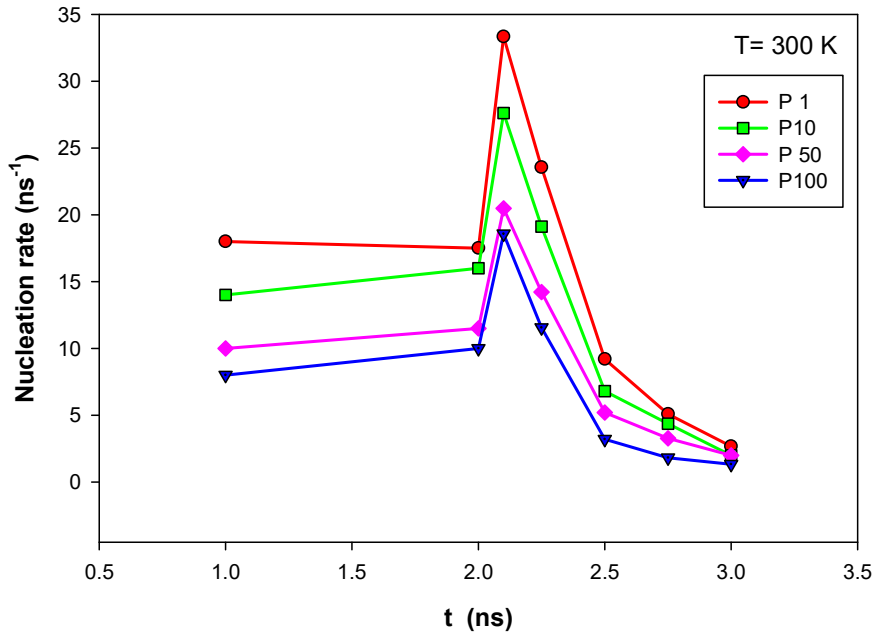


Fig. S6. The nucleation rate at the different temperatures and pressures.

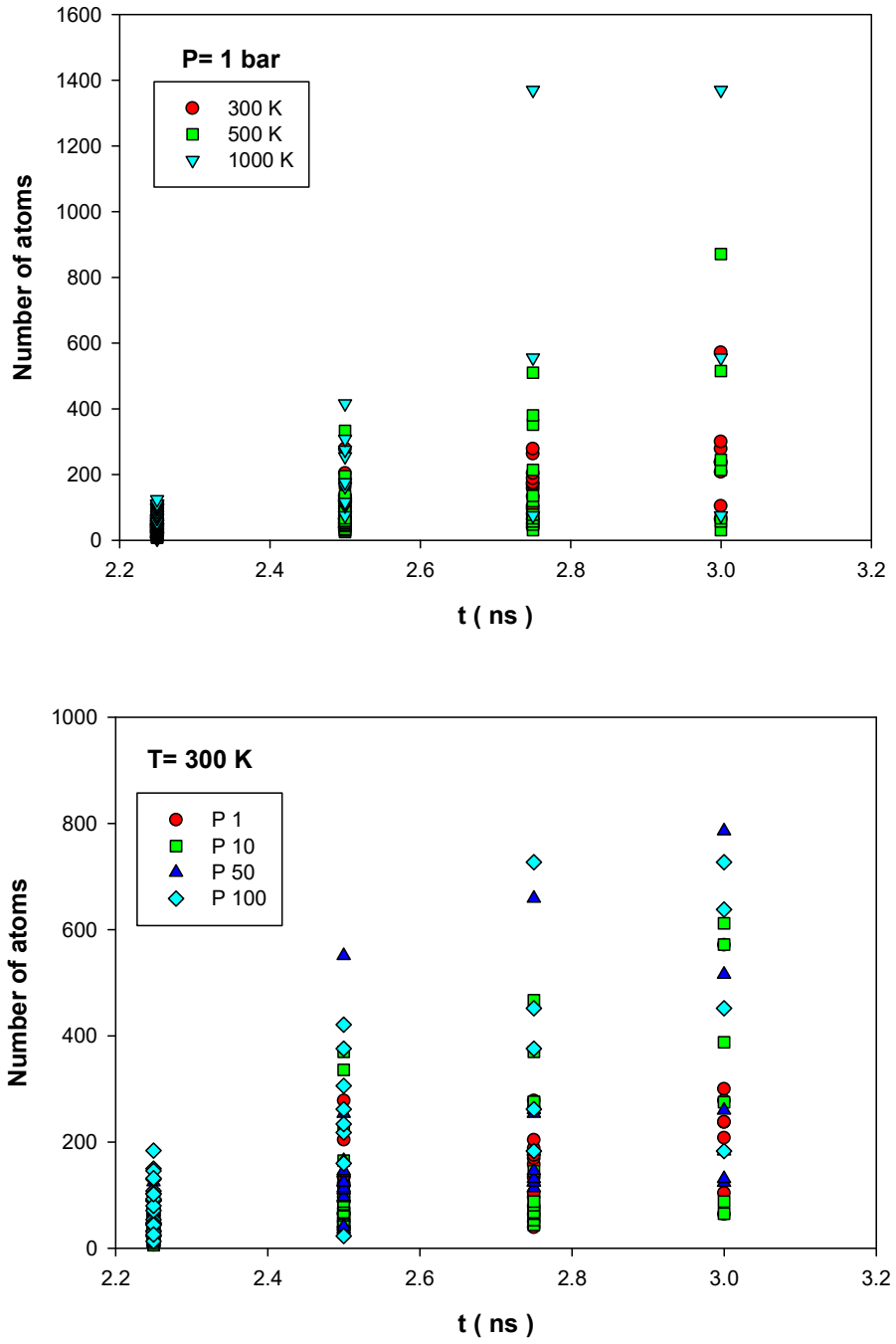


Fig. S7. The number of atoms in the formed clusters at the different temperatures and pressures

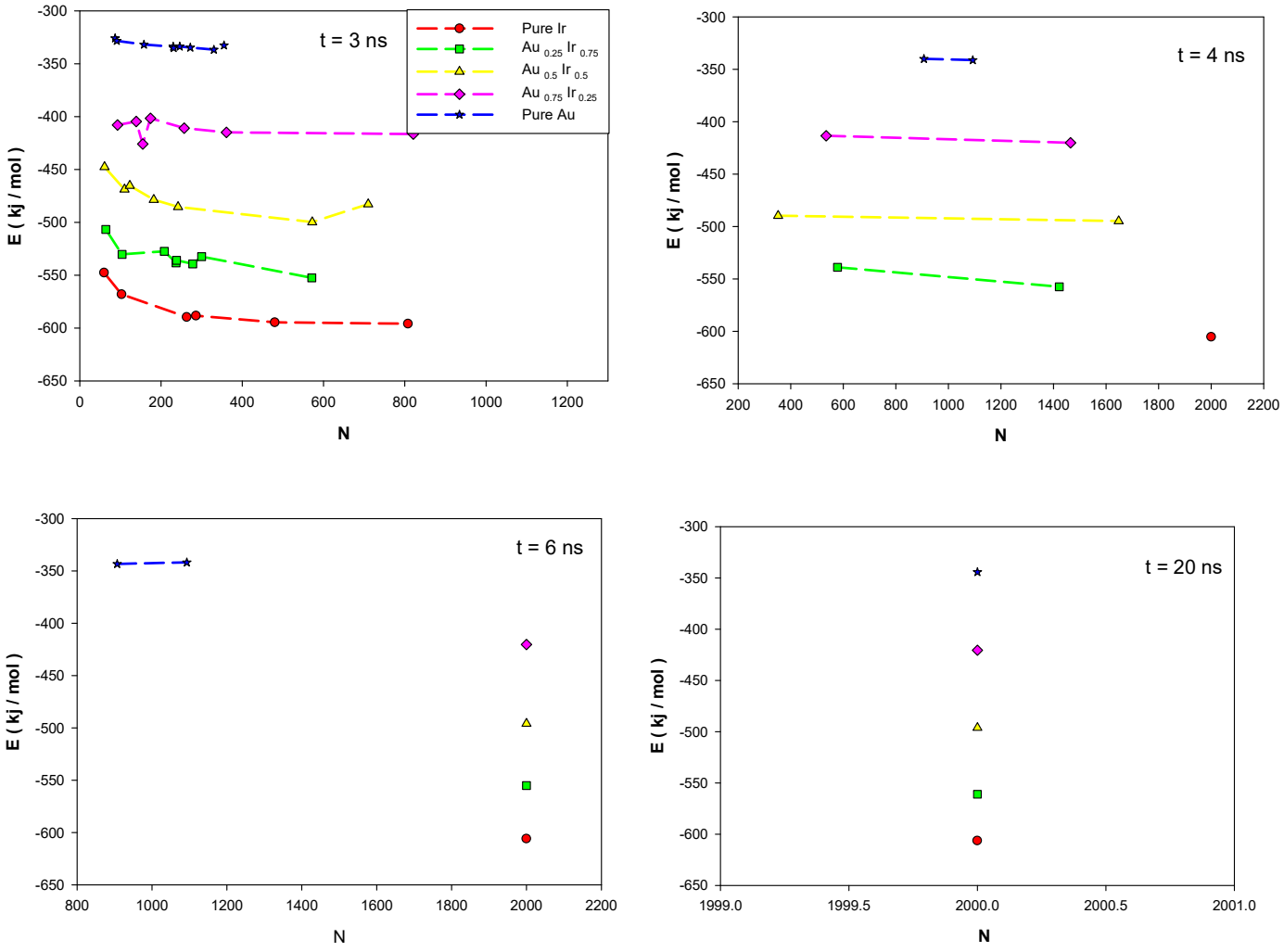


Fig S8. The total energies of the different formed clusters at the different simulation times at 300 K and 1 bar.

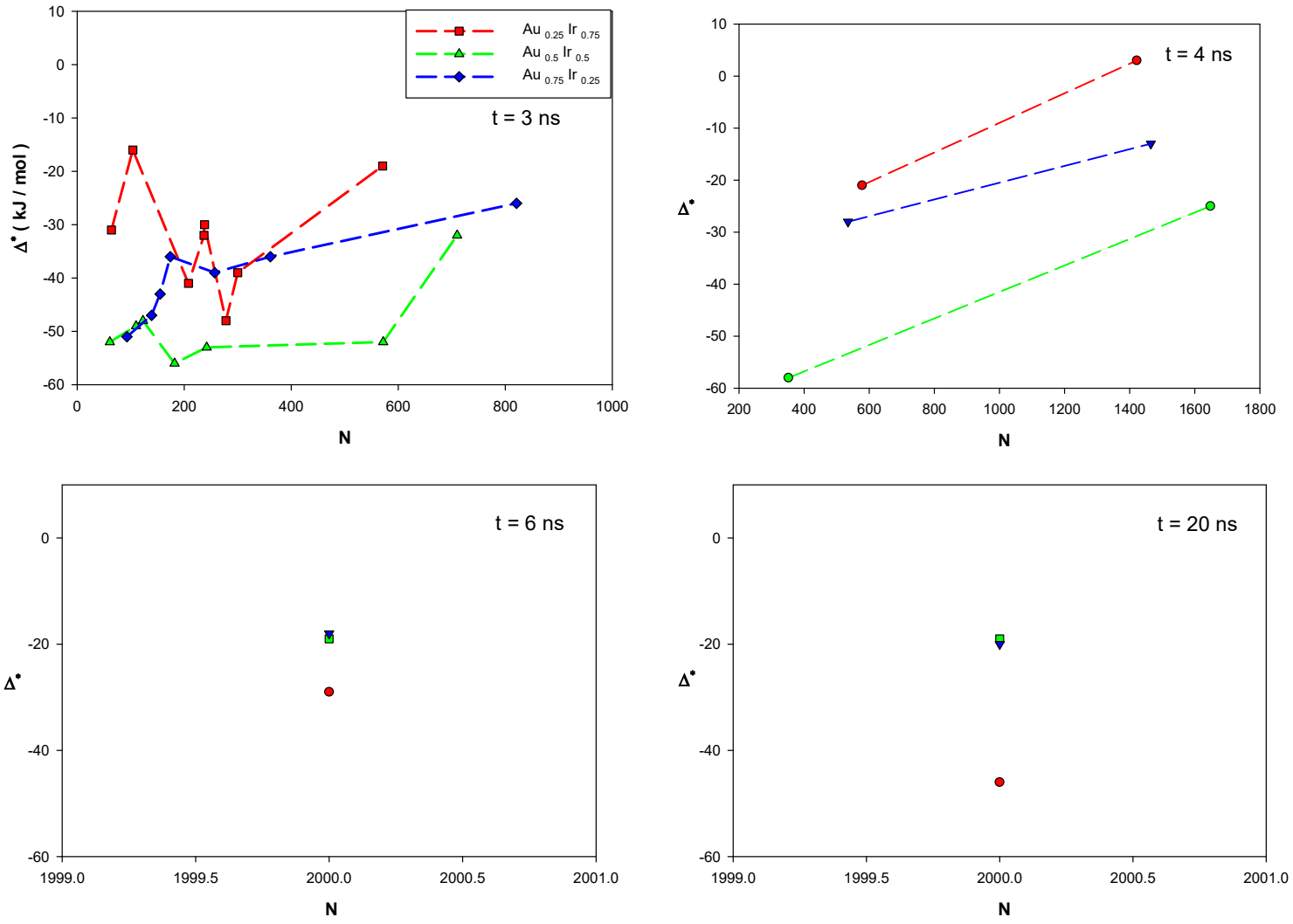


Fig. S9. The Δ^* parameter for the nanoclusters with different Au mole fractions at 300 K and 1 bar at the different simulation times.

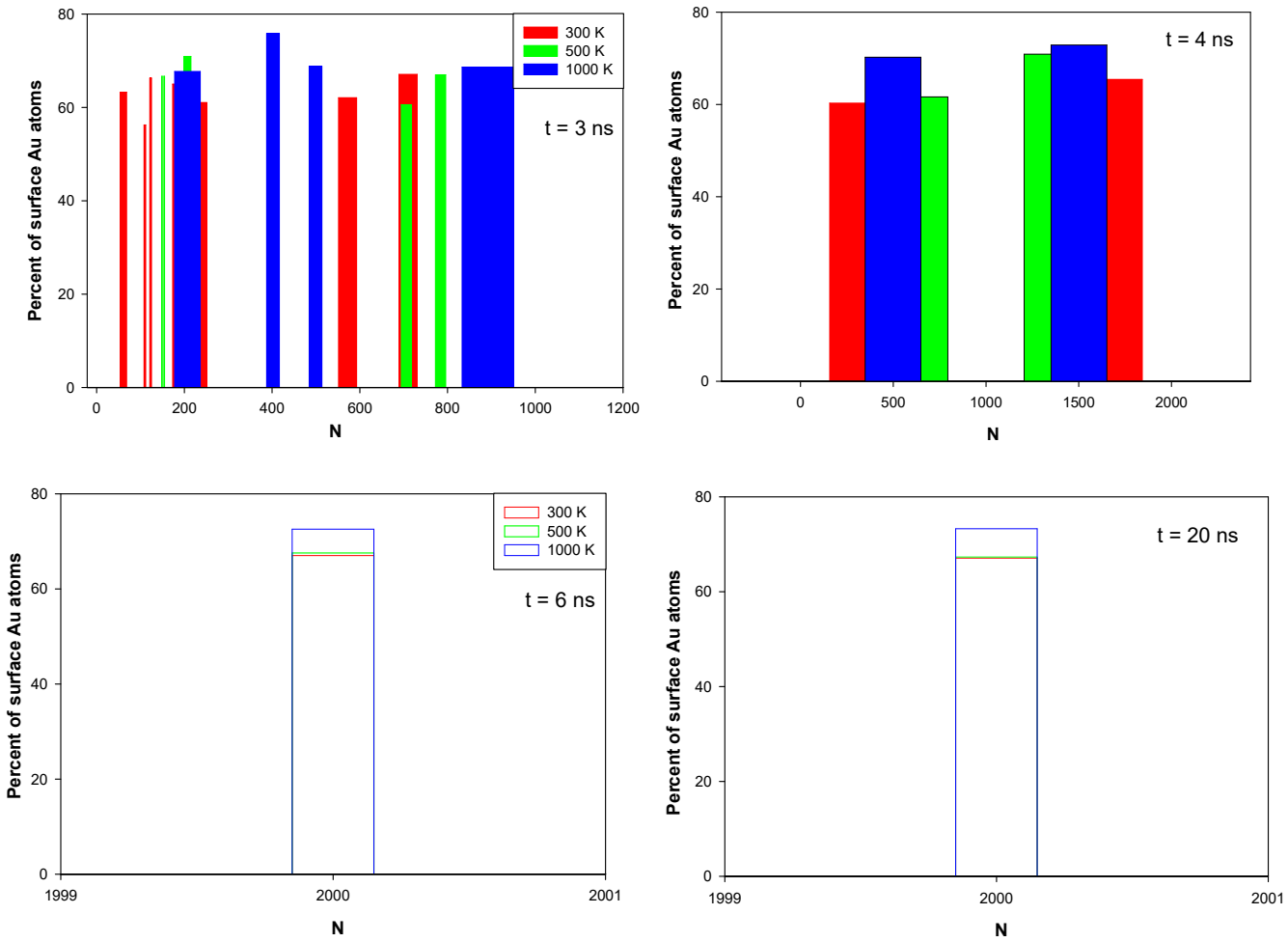


Fig. S10. The percent of the Au atoms on the $Ir_{0.5}Au_{0.5}$ nanoclusters surfaces at 1 bar and different temperatures.

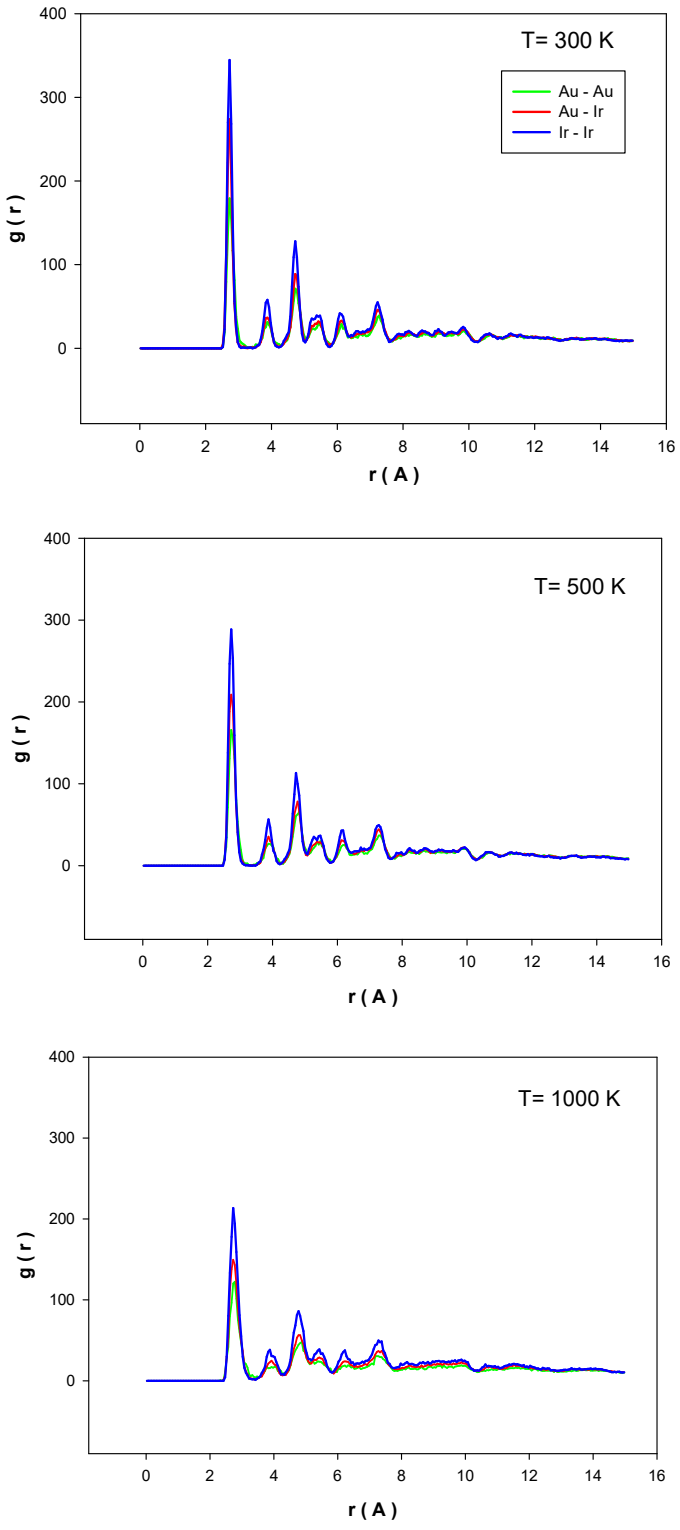


Fig. S11. The Different RDFs for the $Ir_{0.5}Au_{0.5}$ nanoclusters with N= 2000 atoms formed after 20 ns at 1 bar and different temperatures.

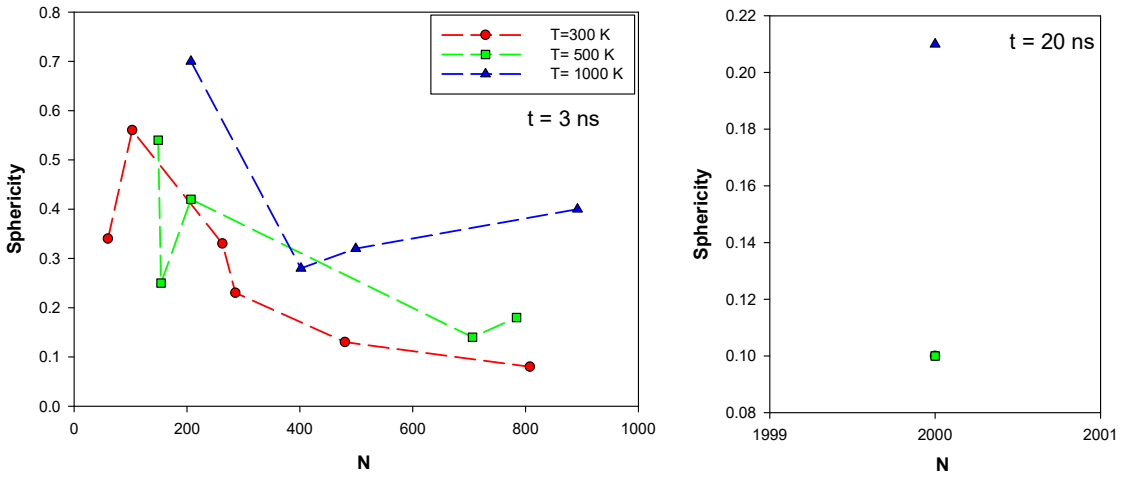


Fig. S12. The sphericity of the $Ir_{0.5}Au_{0.5}$ nanoclusters at 1 bar and different temperatures at 3 and 20 ns.

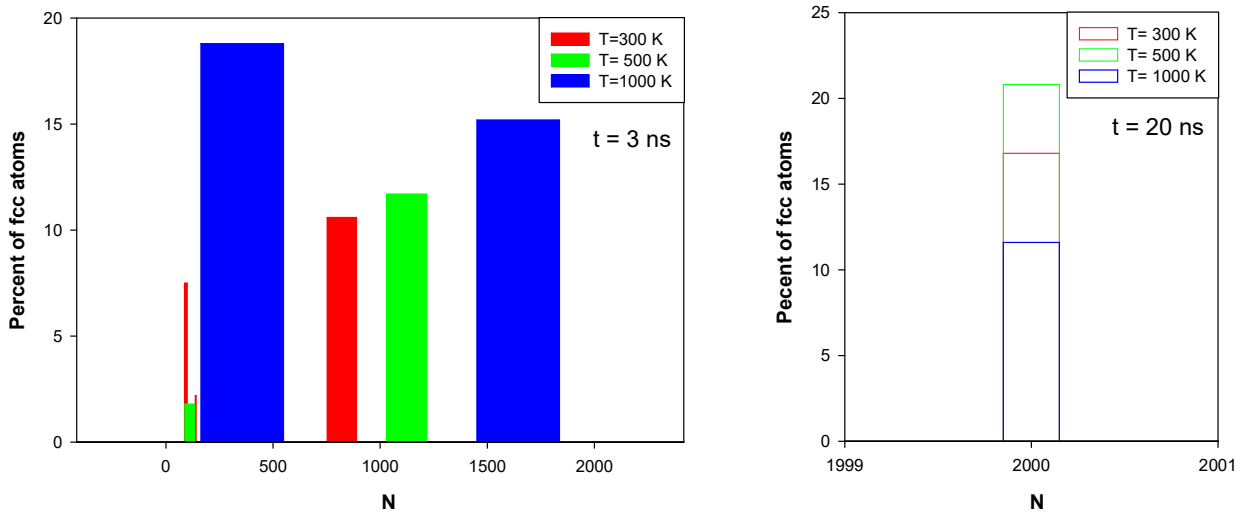


Fig. S13. The percentage of fcc atoms in the $Ir_{0.5}Au_{0.5}$ nanoclusters at 1 bar and different temperatures at 3 and 20 ns.

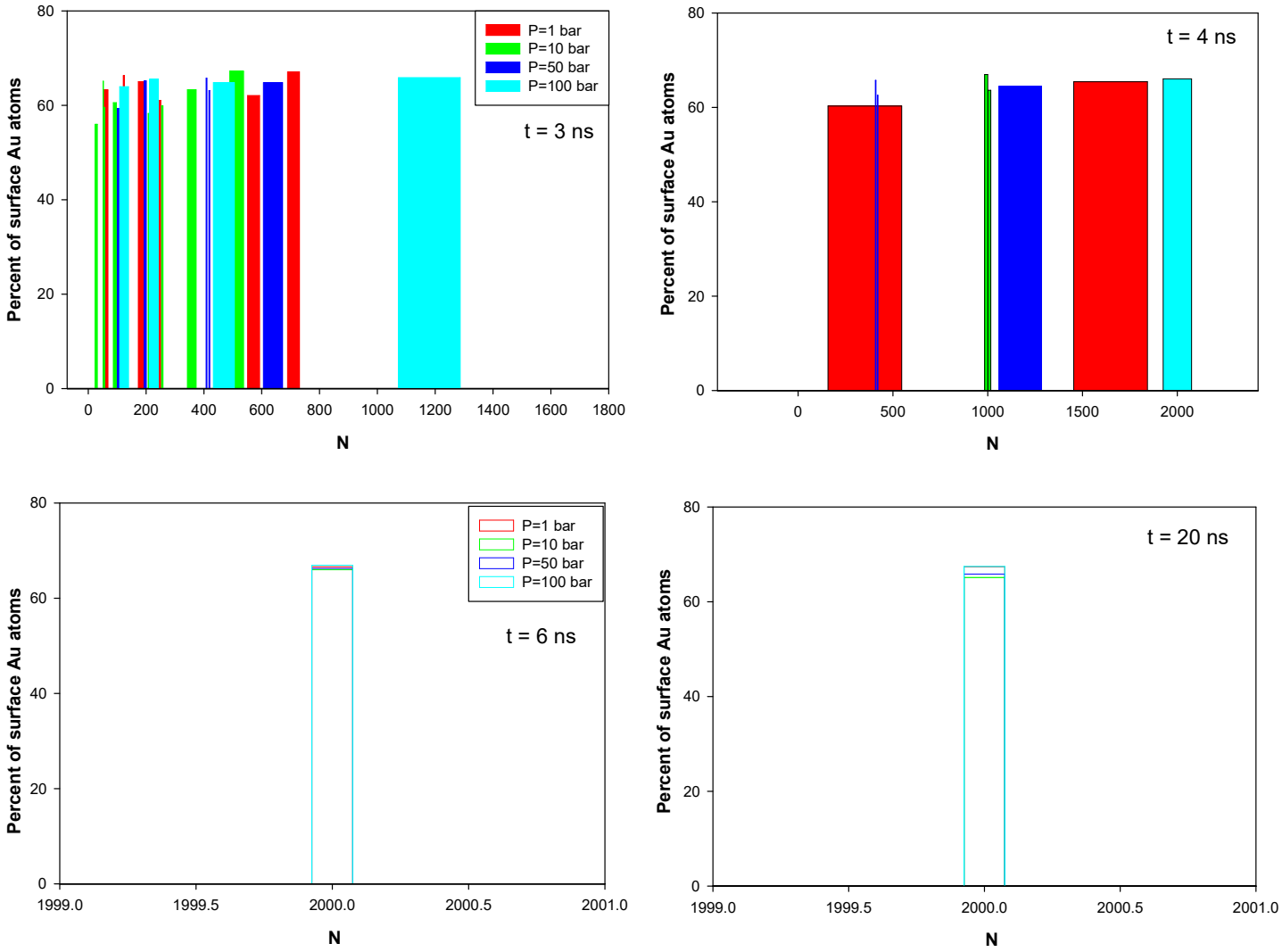


Fig. S14. The percent of the Au atoms on the $Ir_{0.5}Au_{0.5}$ nanoclusters surfaces at 300 K and different pressures.

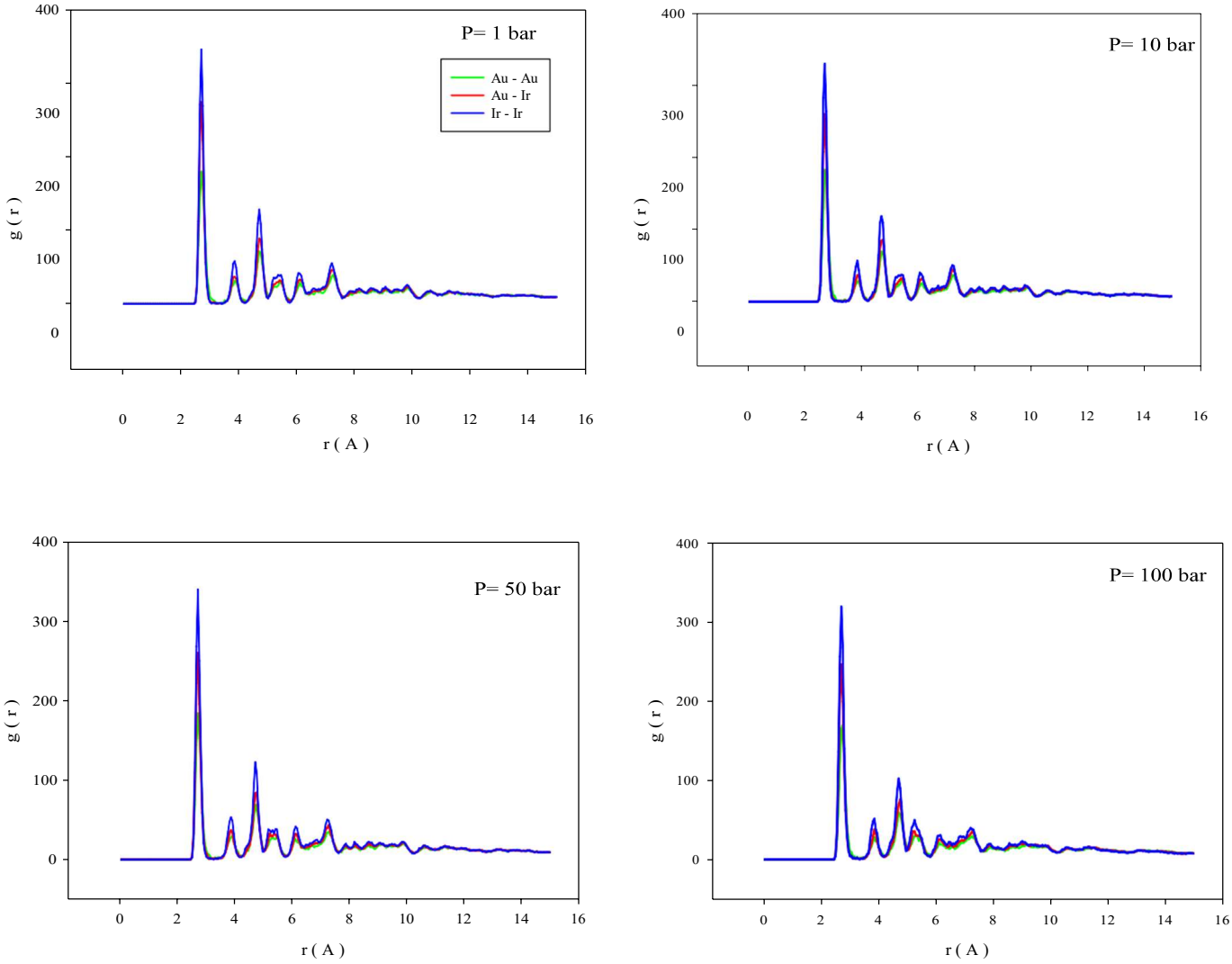


Fig S15. The RDFs of the N=2000 atoms cluster with x_{Au}=0.5 formed at 20 ns at 300 K and different pressures

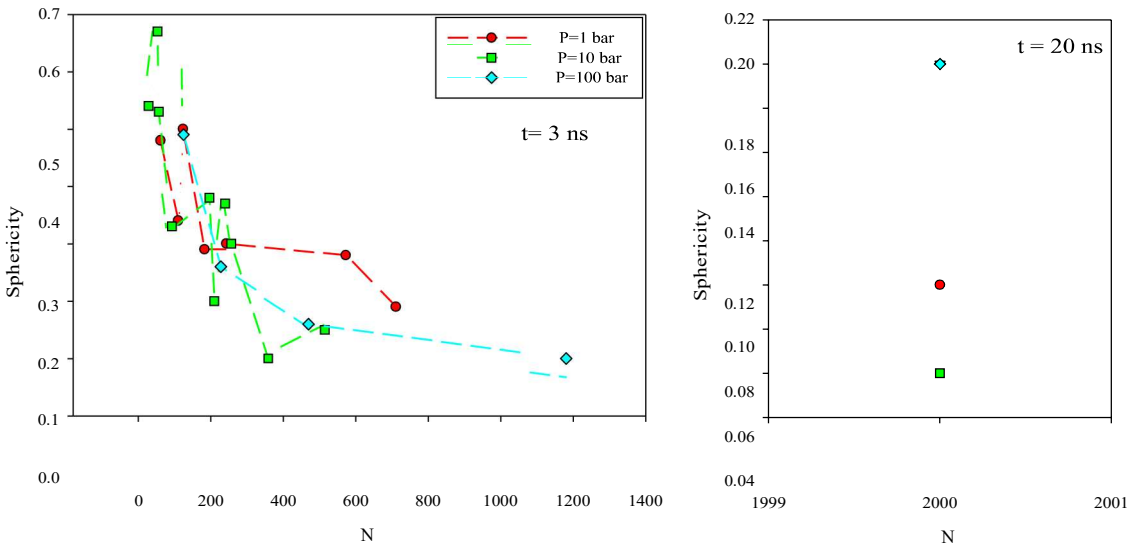


Fig S16. The sphericity of the different clusters with x_{Au}=0.5 formed at 3 and 20 ns at 300 K and different pressures.

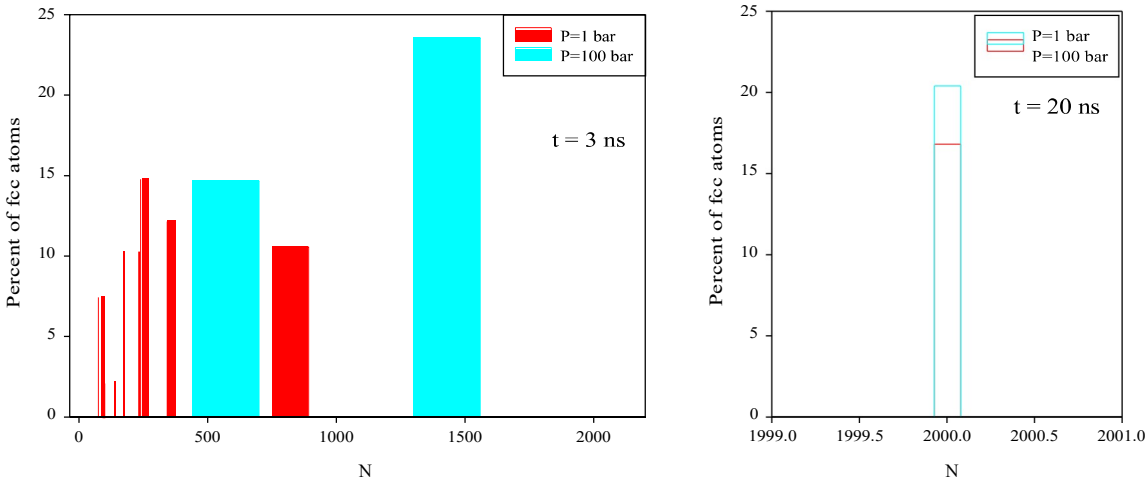


Fig S17. The percent of the fcc atoms in the different clusters with x_{Au}=0.5 formed at 3 and 20 ns at 300 K and lowest and highest pressures.